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A PACKING GENERATION SCHEME FOR THE GRANULAR ASSEMBLIES WITH 3D ELLIPSOIDAL PARTICLES

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SUMMARY

This paper introduces a new generator algorithm and computer program for 3-D numerical simulation of packing configuration in a granular assemblies composed of ellipsoidal particles of different a/b aspect ratios. Each ellipsoidal particle is approximated by the revolution of an ellipse, formed by four connected arcs, about the major axis passing through its centroid. The centroid co-ordinates, major axis direction and lengths of the major and minor axes are the essential data for the packing generation and associated contact detection. The domain to be filled with particles can be a polyhedron of any shape. The packing program was coded based on a newly proposed scheme which obeys the no interpenetration kinematics of solid bodies.

New contact detection algorithms for any two ellipsoids in the packing space were developed. Though simple, these algorithms effectively determine the contact condition and contact point without solving the simultaneous equations of the two ellipsoidal surfaces. Each particle's packing location, contact-point co-ordinates, and three-dimensional graphs can be created using the packing domain given boundaries, along with numbers, and geometrical information of particles to be generated.

Simulation results show that this new algorithm provides an effective packing model as a required initial input for analysing the mechanics of granular material. This generation scheme potentially can explore the complex 3-D behaviours of material composed of discrete particles. Copyright © 1999 John Wiley & Sons, Ltd.

Key words: granule; packing; ellipsoid; contact; algorithm

1. INTRODUCTION

Granular materials are commonly described as a collection of distinct particles that can displace from one another with some degree of independence and which interact basically through contact mechanisms. The discrete nature of such materials establishes non-continuous and discrete load transfer behaviour which can be related to the material microstructure or fabric.[1,2] Packing fabric measures have included branch vectors, normal contact vectors, co-ordination or contact numbers, void characterizations, etc. These fabric measures are determined primarily by the particle shape, packing geometry, particle material and contact surface conditions. In the past, many researchers[1–7] worked on the linkage of fabric to the mechanical response of the particulate media concentrating on describing the packing state and distribution of interparticle contacts. In

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whatever forms such fabric tensors are defined, it is difficult to determine their values by experimental means, because the materials internal structure cannot be observed without disrupting it. Many researchers have avoided this problem by observing artificial 'two-dimensional granular materials' consisting of plates of circle (or oval) shape or rods of circular (or oval) cross-section. A discipline called stereology has been developed to estimate three-dimensional structures from 'two-dimensional observations'. It has been difficult to apply stereology to granular materials because the material is loose and disconnected.

Numerical simulation of granular assemblies has been used for some time to gain insight into micro mechanical behaviour and to facilitate development of a micromechanics-based constitutive model of discrete materials. Unlike physical and analytical modelling, numerical simulation can provide essentially any desired piece of information (stresses, strain, detailed micro-mechanical statistics, and spatial distribution of fabric parameters) at any step during loading. For any numerical simulation of particulate media behaviours, the granular assembly packing is required as the essential input configuration. An automatic packing generator eliminates the researcher need to input geometrical data of the granular congregated medium. Generated packing can also be more similar to natural material.

It is worth pointing out that packing research has focused primarily on developing disk- and sphere-based numerical codes for simplicity, and little has been done with ellipsoidal-shaped particles, BALL,[8] TRUBAL,[9] CONBAL,[10] GLUE[11] and DISC[12] are some available codes for circular-shaped particles. The main drawback of using a monotonous rounded-particle system in modelling real material is that praticle rolling can dominate as a deformational mechanism, resulting in very low shear resistance. Therefore, replacing circular shapes with elliptical shapes has been investigated by some researchers.[13–17] However, it has become evident that the gap between 'two-dimensional materials' and 'three-dimensional materials' is insurmountably wide. The particle ability to change its arrangement, three-dimensionally is essential to the macroscopic behaviour of granular materials. Though various attempts have been made, appropriate means to observe three-dimensional internal microstructures are still unavailable. This is a major obstacle to progress in the micromechanical approach of granular materials.[18] To study the real behaviours of a general particle system, the development of a numerical code based on 3-D ellipsoidal elements has its own meaning.

However, perhaps due to the difficulty in three-dimensional contact detection of ellipsoidal particles and the need for more computational effort, little research result of numerical simulation using ellipsoids has been shown in the past decade. Lin and Ng[19] had proposed two contact-detection algorithms for three-dimensional ellipsoids in discrete element modelling. One algorithm is based on a geometric potential concept, while the other algorithm is based on a common normal concept. Both algorithms require numerically solving either a sixth-order polynomial equation or a set of six simultaneous equations to determine the co-ordinates of two points for contact detection. The accuracy and the efficiency of performing the contact detection are affected by the numerically solving process. But. a 'correct' contact point has hard to define rigorously. Different contact detection results may be obtained by detection schemes with different mathematical considerations. Although the algorithm based on geometric potential has the deficiency of the normal vectors at the calculated contact detection points, may not be parallel to each other. It was still selected by Lin and Ng[20] to develop their DEM code 'ELLIPSE3D' according to the accuracy and efficiency evaluation results between the two algorithms.

This paper presents a packing-generation program called ELLIPSOID, designed for granular assemblies with 3-D ellipsoidal particles. The paper also constructs an approximation of

ellipsoids, based on the four-arc approximation theory of ellipse developed by the first author.[14] One may argue this 3-D work is a natural extension of the previous work[14] by the first author. But, it has to point out that the derivation of the contact detection scheme in 3-D is not straightforward at all. A three-dimensional contact detection theory of any two ellipsoids in space is developed as the core of any 3-D computational method in the particulate mechanics. This algorithm requires no solving of high-order polynomial equation but with more applications of the mathematical theory of geometry. Some simple rules for contact detection are derived and summarized for user to develop one's own numerical simulation code. It is believed that the contact algorithm proposed in this paper can compete with Lin and Ng's algorithms both in the efficiency and the accuracy of numerical simulation.

2. APPROXIMATION OF AN ELLIPSOID

The first author derived a four-arc approximation method of an ellipse with major and minor axes of length $2a$ and $2b$.[14] This method described each ellipse as four connected arcs with unique outward normal and no singularity at any point on the particle boundary. As shown in the Figure 1, point C is the centroid of the ellipse, while points I, J, G, F are the centre of the radius of arcs KAL, LEM, MBH and HDK, respectively. The associate formulae for this approximation method are summarized as follows (see Figure 1):

$$\overline{\mathrm{AC}} = \overline{\mathrm{CB}} = a \tag{1}$$

$$\overline{\mathrm{DC}} = \overline{\mathrm{CE}} = b \tag{2}$$

$$\overline{\mathrm{CG}} = \frac{(a^2 - b^2)c + (a^2 + b^2)d}{2ac} \tag{3}$$

$$\overline{\mathrm{CF}} = \frac{(a^2 - b^2)c + (a^2 + b^2)d}{2bc} \tag{4}$$

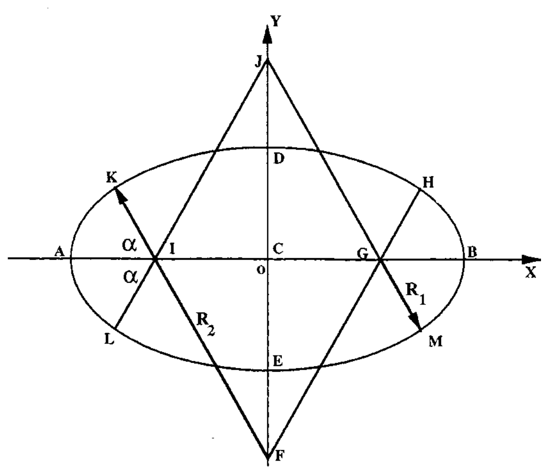


Figure 1. Approximation of an ellipse by four connected arcs

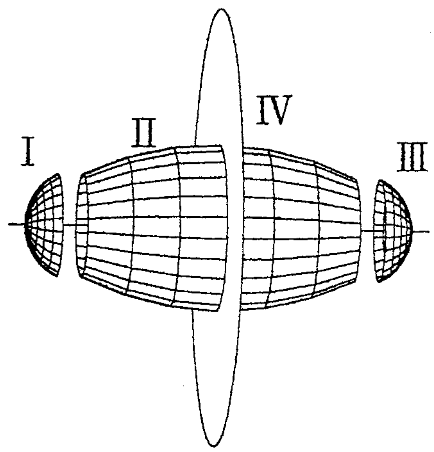


Figure 2. An ellipsoid formed by revolving the four-ac approximated ellipse

where

$$c = \sqrt{a^2 + b^2} \tag{5}$$

$$d = a - b \tag{6}$$

$$\alpha = \tan^{-1}\left(\frac{\overline{\mathrm{CF}}}{\overline{\mathrm{CG}}}\right) = \tan^{-1}\left(\frac{a}{b}\right) \tag{7}$$

$$\overline{\mathrm{GB}} = \overline{\mathrm{GH}} = \overline{\mathrm{GM}} = \overline{\mathrm{AI}} = \overline{\mathrm{AK}} = \overline{\mathrm{AL}} = R_1 = a - \overline{\mathrm{CG}} \tag{8}$$

$$\overline{\mathrm{FK}} = \overline{\mathrm{FD}} = \overline{\mathrm{FH}} = \overline{\mathrm{JL}} = \overline{\mathrm{JE}} = \overline{\mathrm{JM}} = R_2 = b + \overline{\mathrm{CF}} \tag{9}$$

Based on these fundamental equations, the co-ordinates of the end points and centre of radius of each arc for any ellipse in plane translation from the origin with a rotation respect to horizontal axis, can be easily obtained by superimposing the associated rigid-body mode.

A special type of ellipsoid with minor axes of equal length (i.e. $b = c$) can be generated by revolving the major axis of the four-arc approximated ellipse as shown in Figure 2. Though, this is a special type of ellipsoid, it can be used to characterize the main geometrical features of many natural and artificial particles. An ellipsoid, then, is formed by spherical surfaces I and III, and a curved surface II. Surfaces I and III are formed by the revolving of arcs KAL and MBH, respectively, while curved surface II is formed by revolving arcs KH and LM about the major axis. A surrounding ring IV with central axis matching the major axis is formed as the trace of the radius centers J and F during the revolving of the four-arc ellipse. The radius of circle IV is equal to the length of CF as expressed by equation (4). For an ellipsoid in space as shown by Figure 3, major axis directed in $\mathbf{n} = (n_x, n_y, n_z)$, the co-ordinates of a point located on the surrounding ring IV can be derived as

$$x = C_x + r\cos\theta\left(\frac{n_z n_x}{R_{xy}}\right) - r\sin\theta\left(\frac{n_y}{R_{xy}}\right) \tag{10}$$

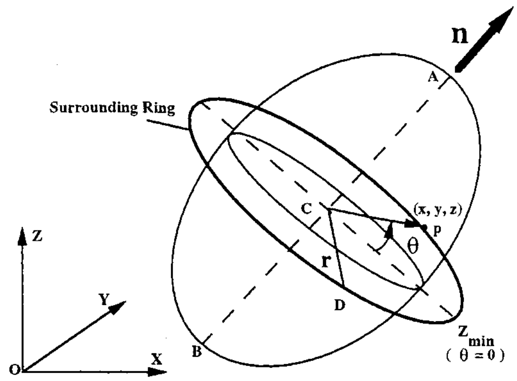


Figure 3. Cartesian co-ordinates of a point p located on the surrounding ring of an ellipsoid in space

$$y = C_y + r\cos\theta\left(\frac{n_z n_y}{R_{xy}}\right) + r\,s\sin\theta\left(\frac{n_x}{R_{xy}}\right) \tag{11}$$

$$z = C_Z - rR_{xy}\cos\theta \tag{12}$$

where the θ is measured counter clockwise from the point with the minimum z co-ordinate and

$$R_{xy} = \sqrt{n_x^2 + n_y^2} \tag{13}$$

$$r = \frac{(a^2 - b^2)\sqrt{a^2 + b^2} + (a^2 + b^2)(a - b)}{2b\sqrt{a^2 + b^2}} \tag{14}$$

Since any point on the ellipsoidal surface has an arc passing through it, the contact detection of any two ellipsoids in the packing space can be easily conducted by checking the distance between the corresponding radius centres. This is the main feature of our contact detection scheme which is different from the other proposed methods[19] of solving complicated geometric equations of 3-D ellipsoids to detect contacts.

3. CONTACT DETECTION

The contact conditions of ellipsoidal particles during motion or packing inside a container can be identified as the following five conditions:

(1) Spherical surface (I or III) of a particle contacts a plane (Figure 4(a)).
(2) Curved surface (II) of a particle contacts a plane (Figure 4(b)).
(3) Spherical surface (I or III) of a particle contacts the spherical surface (I or III) of another particle (Figure 4c).
(4) Spherical surface (I or III) of a particle contacts the curved surface (II) of another particle (Figure 4d).
(5) Curved surface (II) of a particle contacts the curved surface (II) of another particle (Figure 4e).

The contact detection between the two spherical surfaces can be made by comparing the distance between centres with the sum of the radius of the two spheres. The contact detection

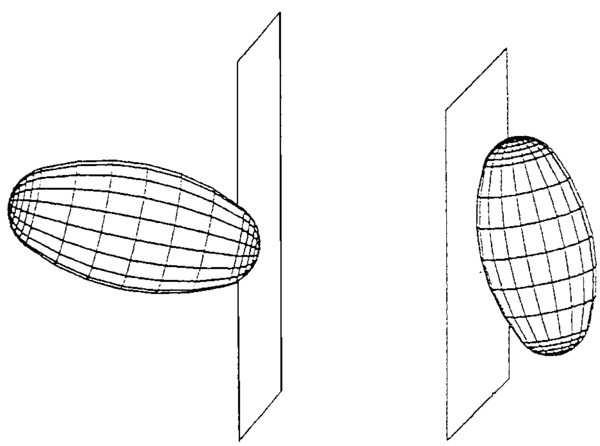
between a sphere and a plane can be conducted by checking the distance of the spherical centre to the plane with the radius of the sphere. Any three-dimensional contact detection related to the curved surface II is somewhat complicated. The curved surface is composed of many arcs with different radius centers. If it can be determined which arc on this surface will contact with the other arc or plane, then the contact detection can be made by comparing the distance between the centre of this arc and the centre of other arc or plane with the impenetrability condition. The contact detection methods between surfaces relating to a curved surface are discussed in the following sections.

3.1. Contact detection between two curved surfaces

Figure 5 shows two curved surfaces from the separate ellipsoids in the packing space contact at point P. Only one tangent plane passes through point P for both curved surfaces. Since both vector AP and vector BP are normal to this tangent plane, one can conclude that the points, A, P and B are on a straight line. Points G and H are the intersection points of line AB with major axis of the ellipsoid, respectively. Points A and B are the centres of the arc passing point P on each curved surface. According to equations (10)–(14), the location of point A (or point B) on the surrounding ring can be determined by only one parameter θ_A (or θ_B). The length of the line AC_1 is equal to the radius of the surrounding arc, so one can determine that the vectors $\mathbf{AC}_1$, $\mathbf{n}_1$ and $\mathbf{AB}$ are on a plane. The same co-plane condition for vectors $\mathbf{BC}_2$, $\mathbf{n}_2$ and $\mathbf{AB}$ can also be obtained. But, it has to point out that the planes AGC_1 and BHC_2 are not necessary to be on the same plane. In general, there are only one edge of each plane, like AG and BH, located on the line AB, while the edges C_1G and C_2H are inclined to each other in the space. From these two properties of co-plane condition, the following two vector equations can be used to find the co-ordinates of points A and B:

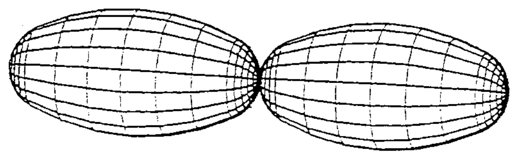
$$(\overline{AC_1} \times \overline{n_1}) \cdot \overline{AB} = 0 \tag{15}$$

$$(\overline{BC_2} \times \overline{n_2}) \cdot \overline{AB} = 0 \tag{16}$$

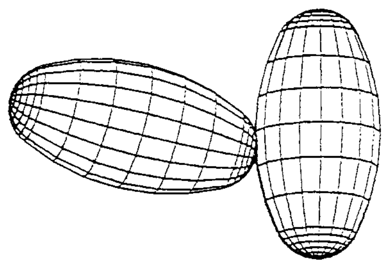


(a) (b)

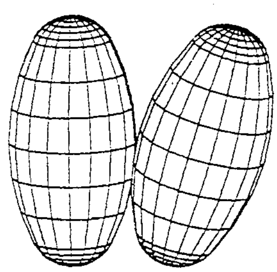
Figure 4. Contact conditions for particles inside a container, (a) sphere–plane (b) curved surface–plane, (c) sphere–sphere, (d) sphere–curved surface, (e) curved surface–curved surface



(c)



(d)



(e)

Figure 4. *Continued.*

After applying equations (10)–(14) into equations (15)–(16), a set of non-linear simultaneous equations of the following form can be determined:

$$a_1 \cos\theta_A + a_2 \sin\theta_A + a_3 \sin\theta_A \sin\theta_B + a_4 \sin\theta_A \cos\theta_B + a_5 \cos\theta_A \sin\theta_B + a_6 \cos\theta_A \cos\theta_B = 0 \tag{17}$$

$$b_1 \cos\theta_B + b_2 \sin\theta_B + b_3 \sin\theta_A \sin\theta_B + b_4 \sin\theta_A \cos\theta_B + b_5 \cos\theta_A \sin\theta_B + b_6 \cos\theta_A \cos\theta_B = 0 \tag{18}$$

where the coefficients $a_i, b_i\,(i = 1, 6)$ are constants determined by the directional cosines of vectors $\mathbf{n}_1$ and $\mathbf{n}_2$ of the major axes, co-ordinates of the centroid of both ellipsoids and the radii of the surrounding rings.

Instead of solving these non-linear equations for θ_A and θ_B, the following iteration method was used to find the positions of A and B on each surrounding ring. As shown by Figure 6, it can be

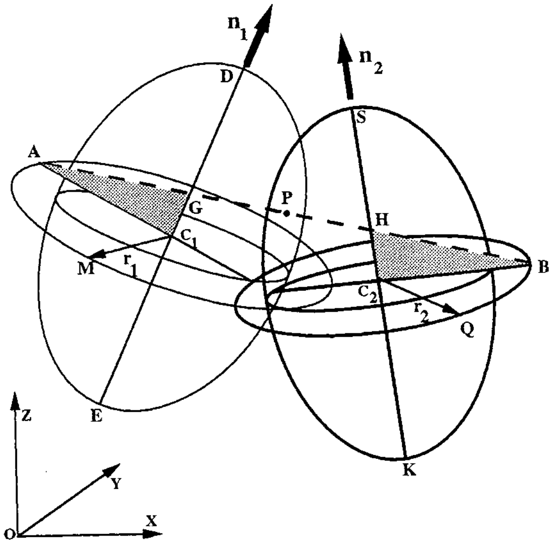


Figure 5. Co-plane conditions of vector set (AB, AC_1, n_1) and vector set (AB, BC_2, n_2), respectively

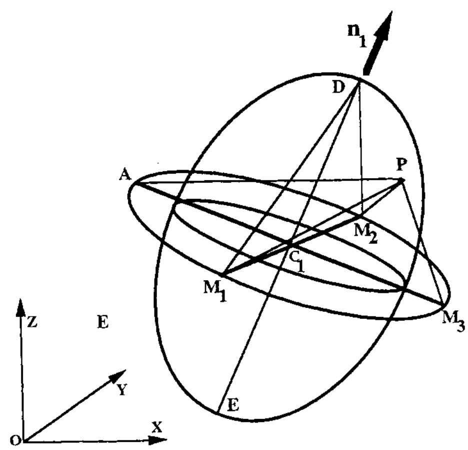


Figure 6. Point on the surrounding ring having largest distance with the contact point P

seen that if point A is the center of the arc passing through the contact point P, then point A is the farthest one to the point P compared with other points located on the surrounding ring. The same conclusion can be drawn for point B on the other surrounding ring. Since points A, P, and B are in a line, then it can be proved that the distance between points A and B in Figure 5 is the largest one among any pair of points selected separately from those two surrounding rings. An iterative method is used to find the pair of points with the longest distance between them. First we choose three points on each ring with 120° divided angle. Then, nine combinations must be evaluated to find the pair ($A^{(1)}$ and $B^{(1)}$) with the longest distance. In the second iteration step, another two

points on each ring are found by adding and subtracting 60° from the co-ordinates $\theta_{A^{(1)}}$ (or $\theta_{B^{(1)}}$) just obtained. Again, the pair of points with the longest distance should be selected from these nine new combinations. After a few iterations, it will converge to two points with the absolute longest distance. For n iteration steps taken, the error is equal to $\pm 60/(2^{(n-1)})^{\circ}$. The value of the longest distance will compare with the sum of the two rings' radii to check whether these two ellipsoids contact. The iteratively determined $\theta_{A^{(n)}}$ and $\theta_{B^{(n)}}$ values have been checked with equations (17) and (18) to verify the iteration scheme accuracy.

3.2. Contact detection of a curved surface with a spherical surface

Figure 7 shows the contact between a spherical surface of ellipsoid C1 and the curved surface of the ellipsoid C2. The point Z is the centre of the sphere and P the contact point of these two ellipsoids. The discussion in the previous section shows that points B, P and Z are on the same line and that point B has the longest distance with point Z. Using the iterative method mentioned in the previous section, the location of point B can be found. The contact condition can be determined by comparing the distance between points Z and B with the sum of the sphere radius and the curved surface arc radius.

3.3. Contact detection of a curved surface with a plane

Figure 8 shows that the ellipsoid contacts a plane at point P. Point C is the ellipsoid centroid and the θ is the angle between the plane normal vector $\mathbf{N}$ and the direction vector $\mathbf{n}$ of the ellipsoid major axis. Figure 8 shows that when the curved surface of an ellipsoid has contact with a plane, the distance between the centroid and the plane is equal to

$$\overline{\mathrm{CH}} = b + \frac{(a^2-b^2)\sqrt{a^2+b^2}+(a^2+b^2)(a-b)}{2b\sqrt{a^2+b^2}}(1-\sin\theta). \tag{19}$$

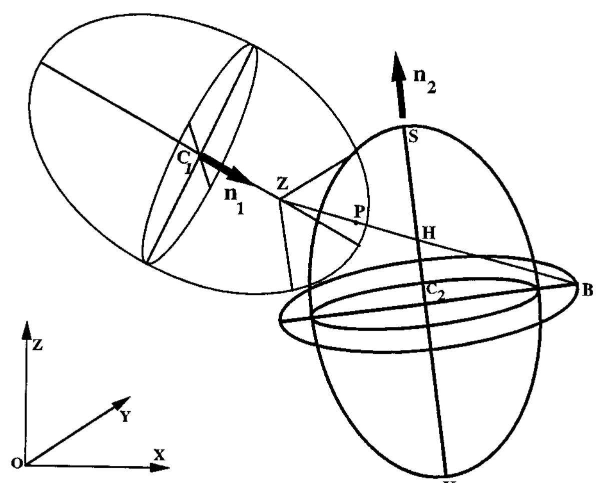


Figure 7. Contact detection between spherical surface and curved surface

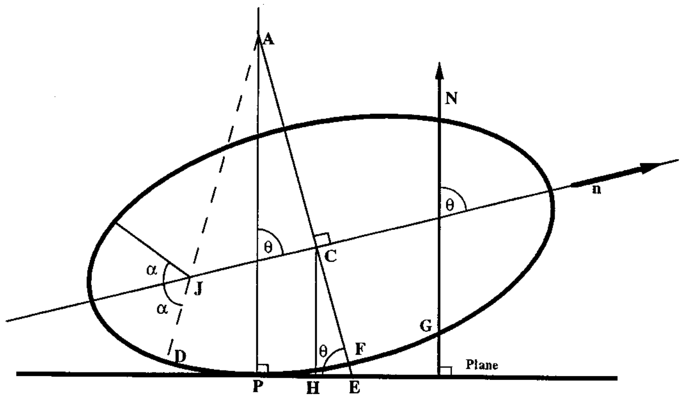


Figure 8. Contact detection between a curved surface and a plane

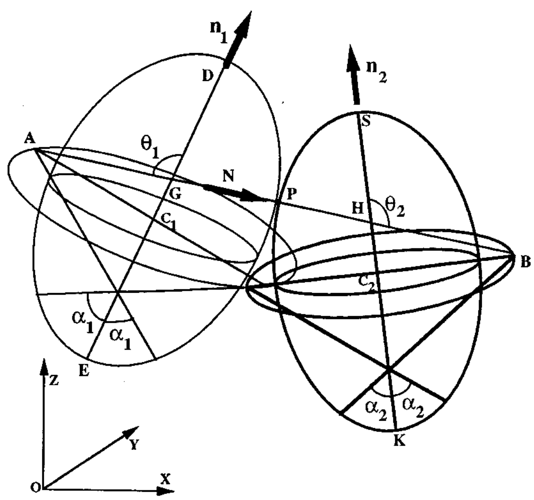


Figure 9. Angles used for the determination of the contact detection type

Then, the contact detection criterion for the curved surface with a plane is the distance between the centroid and the plane with the value obtained from equation (19).

3.4. Determination of the contact detection type

Since there are five types of contact condition that an ellipsoid may admit during packing or motion, some rules will help analysts determine which contact detection type accelerates the simulation speed. Followings are the summarized rules for the determination of contact detection type:

(I) Contact with plane
If θ is defined as the angle θ between the direction vector $\mathbf{n}$ of the major axis and the normal vector $\mathbf{N}$ of the plane (see Figure 8), then
(a) when $\theta > \alpha$, the curve surface of the ellipsoid contacts with the plane,
(b) when $\theta < \alpha$, the spherical surface of the ellipsoid contacts the plane.

(II) Contact between two ellipsoids
For any two ellipsoids in space, the points A and B located on the surrounding ring of separate ellipsoid, with farthest distance can be determined first. Hence, if the angle between the major axis direction and the line AB of each ellipsoid can be calculated (see Figure 9), then
(a) when $\theta_1 > \alpha_1$ and $\theta_2 > \alpha_2$, the curved surface of ellipsoid-1 contacts the curved surface of ellipsoid-2.
(b) when $\theta_1 < \alpha_1$ and $\theta_2 < \alpha_2$, the curved surface of ellipsoid-1 contacts the spherical surface of ellipsoid-2.
(c) when $\theta_1 < \alpha_1$ and $\theta_2 > \alpha_2$, the spherical surface of ellipsoid-1 contacts the curved surface of ellipsoid-2.
(d) when $\theta_1 < \alpha_1$ and $\theta_2 < \alpha_2$, the spherical surface of ellipsoid-1 contacts the spherical surface of ellipsoid-2.

4. IMPLEMENTATION AND EXAMPLE

Based on the theories developed in the previous sections, a computer simulation code ELLIPSOID applying the Auto-CAD-Release 12 version was written. This program contains the following subroutines:

(1) Formation of ellipsoids with different sizes, direction angles, initial translation velocities and angular velocities for the packing generation.
(2) Particles moving (translating and rotating) in the packing space.
(3) Contact detections.
(4) Rest the new coming particle on a packing position by checking the stabilization criteria for a particle against the existed particles and boundary of container.
(5) Find the velocity vector, $\mathbf{v}$, and angular velocity vector $\boldsymbol{\omega}^*$ for unstable particle after each impact. In the packing simulation scheme, the translation velocity vector and the angular velocity vector are changed according to the following equations:

$$\mathbf{v}^* = \mathbf{v} - 2\frac{\boldsymbol{N}\cdot\mathbf{v}}{|\boldsymbol{N}|^2}\boldsymbol{N} \tag{20}$$

$$\boldsymbol{\omega} = \boldsymbol{\omega} + \mathbf{r}\times(\mathbf{N}/|\mathbf{N}|) \tag{21}$$

where $\mathbf{N}$ is the contact normal vector of the incoming ellipsoid between the existed ellipsoid or the boundary; $\mathbf{r}$ is the vector from the centroid of the ellipsoid to the contact point. $\mathbf{v}$ and $\boldsymbol{\omega}$ are the translation and angular velocity vectors, respectively, before impact.

These velocity adjustment mechanisms, without any meaning of kinetic motion in mechanics, are designed just for the ellipsoid moving to another location to check the stabilization criteria. In order to reduce the time required for the particle to be stabilized, the free motion space for the ellipsoid is gradually reduced during the stabilization process.

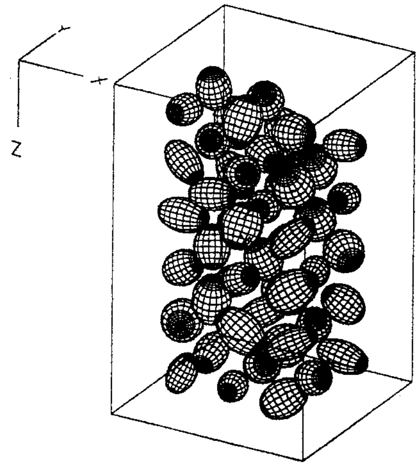


Figure 10. Initial state of 50 freely dropped ellipsoids

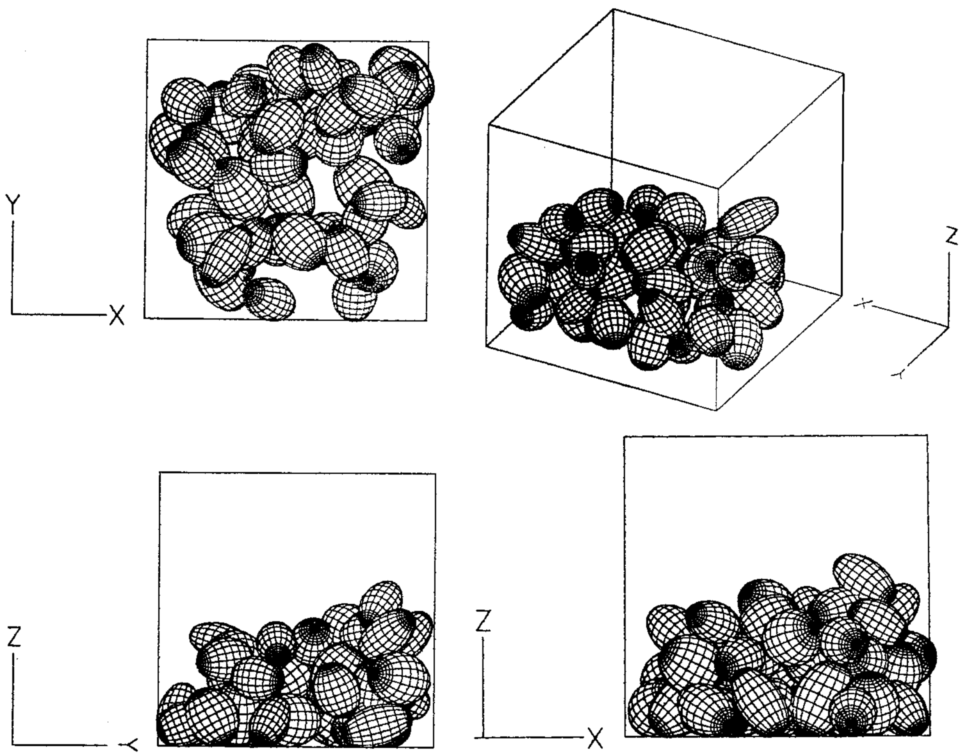


Figure 11. Final packing states viewed from different angles

(6) Output the data (centroid coordinates, direction vectors of major axes, particle sizes, and co-ordinates of contact points).
(7) Graphic displays.

Figures 10 and 11 show the packing process and the final result of 50 ellipsoids inside a box. The packing state can be viewed from different angles. From these figures, it seems that the ELLIPSOID code can generate a reasonable packing configuration. Based on the scheme proposed by this paper, large random particle media assemblies can be numerically generated to study the 3-D behaviours of granular materials. Different researchers may have their own algorithms to generate the packing structures, but the contact detection algorithms proposed by this paper can be considered as a possible solution in the program.

5. DISCUSSION AND CONCLUSIONS

Granular materials mechanics' ultimate purpose is to establish relationships among macroscopic quantities, such as load and deformation, of the material in question. This paper presents—a packing scheme for 3-D ellipsoidal particles that provides researchers with an effective tool to observe three-dimensional internal microstructure varying under deformation. The ellipsoids are formed by a revolving four-arc approximated ellipse about its major axis. This mechanism can generate many different particle shapes observed in natural materials. All contact detection is based on a comparison of distance between the arcs and the associated impenetrability condition. Methods of finding the corresponding arcs to check contact are presented in detail. These contact-detection algorithms are efficient compared with solving the highly non-linear geometrical equations of ellipsoids in 3-D space. Packing ellipsoids with different shapes and sizes can be generated within a given space. The generated packing configuration can be used as the initial state for the numerical analysis of granular material behaviours. This packing generation scheme can also be applied in stereology research of granular materials to understand the internal material structures, such as the average number of particles per unit volume, the distributions of particle size, and the estimation of the structural anisotropy.

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